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Conformational isomerism in 3,5,8-trioxabicyclo[5.1.0]octane and its diastereomeric 4-methyl derivatives. A combined IR, X-ray and ab initio study

A.E. Klimovitskii [a], E.E. Zvereva [b], G.A. Chmutova [a], A.B. Dobrynin [b], V.Yu. Fedorenko [a], Yu.G. Shtyrlin [a], I.A. Litvinov [b], T.V. Bulygina [a], E.N. Klimovitskii [a,*]

[a] *A.M. Butlerov Chemical Institute, Kazan State University, Kazan 420111, Box 115, Russian Federation*
[b] *A.E. Arbuzov Institute of Organic and Physical Chemistry, Russian Academy of Sciences, Arbuzov Str. 8, Kazan 420088, Russian Federation*

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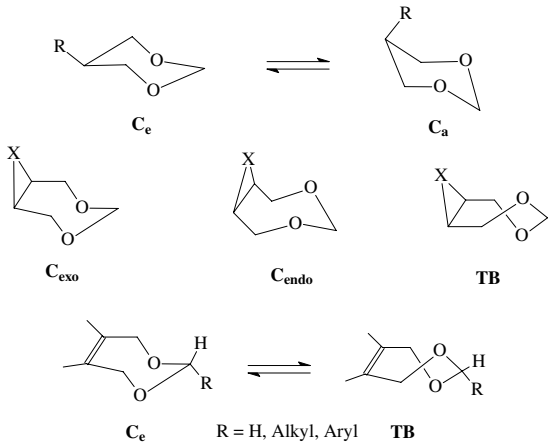
Abstract

IR spectroscopy and ab initio calculations have been applied to the title compounds. Bicyclic acetals were found to exist as mixture of chair and twist-boat conformations, a parent epoxide being in ternary equilibrium. X-ray data on 4-methyl (exo) derivative display a twist-boat form.

Keywords: Seven-membered bicyclic acetals; IR spectroscopy; X-ray crystallography; ab initio calculations

1. Introduction

Investigations of 1,3-dioxanes with substituent at C^5 (polar especially) show a number of interesting trends [1]. 3,5-Dioxabicyclo[5.1.0]octanes with exo- and endo chair-like conformations relate closely to above 1,3-dioxanes if one assumes that three-membered cycles in these molecules are equivalent to substituents at C^5 in the stereochemical sence (axial ≡ endo and equatorial ≡ exo). The noticeable feature of bicyclic acetals is the real propensity to exist in both chair conformations and a twist-boat form in addition [2–9]. It is worth noting that seven-membered acetals with a planar fragment have been inspected thoroughly and untraditional chair–twist-boat (C ⇌ TB) equilibrium has been clarified [10].



One can expect that bicyclic acetals with X = C, O, S, N may serve as suitable models for the investigation of polar and steric interactions between acetal moiety and three-membered rings. Encouraged by available stereochemical information implying both a broad range of

* Corresponding author. Fax: +7 8432 9272 78.
E-mail address: evgenii.klimovitskii@ksu.ru (E.N. Klimovitskii).

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